

Phthalic acid, 2,4-dichlorobenzyl nonyl ester

Inchi:	InChI=1S/C24H28Cl2O4/c1-2-3-4-5-6-7-10-15-29-23(27)20-11-8-9-12-21(20)24(28)30-1
InchiKey:	CXEDXLICTVHBCL-UHFFFAOYSA-N
Formula:	C24H28Cl2O4
SMILES:	CCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	451.38

Physical Properties

Property code	Value	Unit	Source
gf	-144.57	kJ/mol	Joback Method
hf	-621.12	kJ/mol	Joback Method
hfus	58.80	kJ/mol	Joback Method
hvap	102.64	kJ/mol	Joback Method
log10ws	-8.79		Crippen Method
logp	7.258		Crippen Method
mcvol	340.860	ml/mol	McGowan Method
pc	1199.79	kPa	Joback Method
rinpol	3096.00		NIST Webbook
rinpol	3096.00		NIST Webbook
tb	1044.26	K	Joback Method
tc	1280.83	K	Joback Method
tf	654.80	K	Joback Method
vc	1.310	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1057.56	J/mol×K	1044.26	Joback Method
cpg	1069.02	J/mol×K	1083.69	Joback Method
cpg	1079.02	J/mol×K	1123.12	Joback Method
cpg	1087.63	J/mol×K	1162.54	Joback Method
cpg	1094.89	J/mol×K	1201.97	Joback Method
cpg	1100.85	J/mol×K	1241.40	Joback Method
cpg	1105.58	J/mol×K	1280.83	Joback Method
dvisc	0.0001817	Paxs	654.80	Joback Method

dvisc	0.0001113	Paxs	719.71	Joback Method
dvisc	0.0000739	Paxs	784.62	Joback Method
dvisc	0.0000522	Paxs	849.53	Joback Method
dvisc	0.0000388	Paxs	914.44	Joback Method
dvisc	0.0000299	Paxs	979.35	Joback Method
dvisc	0.0000239	Paxs	1044.26	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382565&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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